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INTERPRETING A HANDBOOK

You should look up information concerning any organic chemical you'll be working with so that you know what to expect in terms of molecular weight, density, solubility, crystalline form, melting or boiling point, color, and so on. This information is kept in handbooks that should be available in the lab, if not in the library. Reading some of these handbooks is not easy, but once someone tells you what some of the fancy symbols mean, there shouldn't be a problem. Many of the symbols are common to all handbooks and are discussed only once, so read the entire section even if your handbook is different. There are at least four fairly popular handbooks, and I've included sample entries of 1-bromobutane and benzoic acid, a liquid and a solid you might come across in lab, to help explain things.

CRC HANDBOOK

(**CRC Handbook of Chemistry and Physics**, CRC Press, Inc., Boca Raton, Florida.) Commonly called "the CRC" as in "Look it up in the CRC." A very popular book; a classic. Sometimes you can get the last year's edition cheaply from the publisher, but it's usually for an order of 10 or more.

Entry: 1-Bromobutane (Fig. 11)

1. **No. 3683.** An internal reference number. Other tables in the handbook will use this number rather than the name.
2. **Name,...Butane, 1-bromo.** You get a systematic name and a formula.
3. **Mol. wt. 137.03.** The molecular weight of 1-bromobutane.
4. **Color,... ..** Dots! This implies 1-bromobutane is a colorless liquid: nothing special really.
5. **b.p. 101.6, 18.8³⁰.** The normal boiling point, at 760 torr, is 101.6°C. The 18.8 has a tiny superscript to tell you that 18.8°C is the boiling point at 30 torr.
6. **m.p. -112.4.** The melting point of solid 1-bromobutane. Handbooks report only the TOP of the melting point range. You, however, should report the *entire* range.
7. **Density. 1.2758^{20/4}.** Actually, this particular number is a **specific gravity**. This is a mass of the density of the liquid taken at 20°C referred to (divided by) the density of the same mass of water at 4°C.

PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS (Continued)

No.	Name, Synonyms, and Formula	Mol. wt.	Color, crystalline form, specific rotation and λ_{max} (log ϵ)	b.p. °C	m.p. °C	Density	nd	Solubility	Ref.
2531	Benzoic acid $\text{C}_6\text{H}_5\text{CO}_2\text{H}$	122.13	mel lf or nd	249, 133 ¹⁰	122.13	1.0749 ³⁰ 1.2659 ^{3/4}	1.504 ¹²	al, eth, ace, bz, chl	B9 ³ , 360
2532	Benzoic acid, 2-acetamido $2\text{-(CH}_3\text{CONH)C}_6\text{H}_4\text{CO}_2\text{H}$	179.18	nd (aa)		185			eth, ace, bz	B14 ³ , 922
3683	Butane, 1-bromo $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$	137.03		101.6, 18.8 ³⁰	-112.4	1.2758 ^{30/4}	1.440 ²⁰	al, eth, ace, chl	B1 ⁴ , 258
3684	Butane, 1-bromo-4-chloro $\text{BrCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$	171.48		174-57 ³⁶ , 63-4 ¹⁰		1.488 ^{30/4}	1.4885 ²⁰	al, eth, chl	B1 ⁴ , 264

Fig. 11 Sample CRC entries from the 61st edition.

That's what the tiny 20/4 means. Notice the units will cancel. A number without the modifying fraction is a true density (in g/ml) at the temperature given.

8. **n_D 1.4401²⁰**. This is the index of refraction (see Chapter 28, "Refractometry") obtained using the yellow light from a sodium lamp (the D line). Yes, the tiny 20 means it was taken at 20°C.
9. **Solubility. al, eth, ace, chl**. This is what 1-bromobutane must be soluble in. There are a lot of solvents, and here are the abbreviations for some of them:

al	alcohol	eth	ether
bz	benzene	chl	chloroform
peth	petroleum ether	w	water
aa	acetic acid	MeOH	methanol
lig	ligroin	CCl ₄	carbon tetrachloride
to	toluene	ace	acetone

Some solvents have such a long tradition of use, they are our old friends and we use very informal names for them:

alcohol. Ethyl alcohol; ethanol.

ether. Diethyl ether; ethoxyethane.

pet. ether. Petroleum ether. Not a true ether, but a low-boiling (30–60°C) hydrocarbon fraction like gasoline.

ligroin. Another hydrocarbon mixture with a higher boiling range (60–90°C) than pet. ether.

10. **Ref. B1⁴ 258**. Reference to listing in a set of German handbooks called Beilstein. Pronounce the German "ei" like the long i, and stop yourself from saying "Beelsteen" or some such nonsense. 1-Bromobutane is in the fourth supplement (⁴), Volume 1 (B1), on page 258.

Entry: Benzoic Acid (Fig. 11)

There are a few differences in the entries, what with benzoic acid being a solid, and I'll point these out. If I don't reexamine a heading, see the explanation back in the 1-Bromobutane entry for details.

1. **Color, ...mcl lf or nd.** Monoclinic leaflets or needles. This is the shape of the crystals. There are many different crystalline shapes and colors, and I can't list them all—but here's a few:

pl	plates	mcl	monoclinic
nd	needles	rh	rhombus
lf	leaves	ye	yellow
pr	prisms	pa	pale

I've included #2532 (benzoic acid, 2-acetamido) to show that you sometimes get a bonus. Here nd(aa) means you get needle-like crystals from acetic acid. Acetic acid (aa) is the recrystallization solvent (see Chapter 13, "Recrystallization"), and you don't have to find it on your own. Thus, pa ye nd (al) means that pale yellow needles are obtained when you recrystallize the compound from ethanol.

2. **Density. 1.0749¹³⁰.** This is an actual **density** of benzoic acid taken at 130°C. There is no temperature ratio as there is for the specific gravity (1.2659^{15/4}).

Nostalgia

I've included the entries from the 43rd and 49th editions of the *CRC* to show you that not all things improve with age.

1. **General Organization.** The 43rd and 49th editions make use of **boldface type** to list parent compounds and lighter type to list derivatives. Benzoic acid is a parent; there are many derivatives (Fig. 12). The 61st edition lists all compounds with the same weight (Fig. 11).
2. **Solubility tables.** Here the older editions *really* shine. The 43rd edition gives numerical solubility data for benzoic acid: 0.18⁴, 0.27¹⁸, 2.2⁷⁵. These are the actual solubilities, in grams of benzoic acid per 100 g of water at 4, 18, and 75°C, respectively. The butyl bromide (1-bromobutane) entry has helpful solubility indicators: **i.** *insoluble* in water; [8], *miscible* in alcohol; [8], *miscible* in diethyl ether.

Other popular abbreviations for the solubility of a compound are

s	soluble	i	insoluble
δ	slightly soluble		miscible, mixes in all proportions
h	solvent must be hot	v	very

PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS (Continued)

No.	Name	Synonyms and Formula	Mol. wt.	Crystalline form, color and specific rotation	m.p. °C	b.p. °C	Density	n _D	Solubility						Ref.
									w	al	eth	ace	bz	other solvents	
b1239	Benzoic acid . .	Benzenecarboxylic acid. </													

Fig. 12 Sample CRC entries from the 49th edition.

What a big change from the 43rd to the 61st edition. Numerical solubility data missing, solubility indications gone, and even incomplete solubility reporting (Benzoic acid: chl, CCl_4 , acet., me. al., bz, CS_2 —43rd ed.; where are CCl_4 , me. al., and CS_2 in the 61st?). The decrease in organizational structure, I can live with. But the new way of presenting the solubility data (what there is of it) is useless for many things you need to do in your lab. Reread the sample synthesis experiment (see Chapter 2, “Keeping a Notebook”). You need more useful solubility data for that experiment than you can extract from the most recent *CRC Handbook*. For my money, you want a fancy \$17.50 doorstop, get a *CRC* 61st and up. You want useful information, get a *CRC* 60th and back. Or consult the handbook I want to talk about next.

LANGE'S

(**Lange's Handbook of Chemistry**, McGraw-Hill Book Company, New York, New York.) A fairly well-known but not well-used handbook. The entries are similar to those in the *CRC Handbooks*, so I'll only point out the interesting differences.

Entry: 1-Bromobutane (Fig. 14)

1. **Name.** *Butyl bromide(n)*. Here, 1-bromobutane is listed as a substituted butyl group much like it is in the 43rd *CRC*. The systematic name is listed under synonyms.
2. **Beil. Ref. I-119.** The Beilstein reference; Volume 1, page 119, the original work (not a supplement).
3. **Crystalline form . . . lq.** It's a liquid.
4. **Specific gravity 1.275^{20/4}.** The tiny temperature notation is presented a bit differently, but the meaning is the same.
5. **Solubility in 100 parts water. 0.06¹⁶.** 0.06 g of 1-bromobutane will dissolve in 100 g of water at 16°C. After that, no more.

Entry: Benzoic Acid (Fig. 14)

1. **Melting point. subl^{>=} 100.** Benzoic acid starts to **sublime** (go directly from a solid to a vapor) over 100°C, before any crystals left melt at 122.4°C.

PHYSICAL CONSTANTS OF

No.	Name	Synonyms	Formula	Mol. Wt.
1449	Benzoic acid . . .	benzenecarboxylic acid*; phenylformic acid	C_6H_5COOH	122.12
1450	—, allyl ester. . .	allyl benzoate	$C_6H_5COOC_3H_5$. .	162.18
1451	—, anhydride. . .	See <i>Benzoic anhydride</i> .		
1452	—, benzyl ester .	benzyl benzoate; benzyl benzenecarboxylate	$C_6H_5COOCH_2C_6H_5$	212.24

*Name approved by the International Union of Chemistry.

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PHYSICAL CONSTANTS OF

No.	Name	Synonyms	Formula	Mol. Wt.
2160	Butyl bromide (<i>n</i>) . .	1-bromobutane*	$CH_3(CH_2)_3CH_2Br$.	137.03
2161	<i>sec</i> -Butyl bromide . .	2-bromobutane*; methyl-ethylbromomethane	$C_2H_5CH(CH_3)Br$.	137.03
2162	<i>tert</i> -Butyl bromide .	2-bromo-2-methylpropane*; trimethylbromomethane	$(CH_3)_3CBr$	137.03

*Name approved by the International Union of Chemistry.

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Fig. 13 Sample *CRC* entries from the 41st edition.

2. **Crystalline form...**, *mn.pr.* Monoclinic prisms. Here, *mn* is a variant of the *mcl* abbreviation used in the *CRC*. Don't let these small differences throw you. A secret is that all handbooks have a listing of abbreviations at the front of the tables. Shhhh! Don't tell *anyone*. It's a secret.

I like the *Lange's* format, redolent of the 43rd edition of the *CRC*. The one with the useful information. The organization based on common names,

ORGANIC COMPOUNDS (Continued)

No.	Crystalline form, color and index of refraction	Density g/ml	Melting point, °C	Boiling point, °C	Solubility in grams per 100 ml of		
					Water	Alcohol	Ether, etc.
1449	col. monoc. leaf. or need., 1.53974 ¹⁵	1.2659 ⁴	122	249	0.18 ⁴ 0.27 ¹⁸ 2.2 ²⁵	47.1 ¹⁵	40 ¹⁵ eth.; s. chl., CCl ₃ , acet., me. al., bz., CS ₂
1450	yel. liq.	1.058 ¹³		230	i.	s.	∞ eth.
1451							
1452	col. oily liq., or need. or leaf., 1.5681 ²¹	1.114 ¹⁸	21 (18.5)	323-4 (316-7)	i.	s.	s. eth., chl.; i. glyc.

For explanations and abbreviations see beginning of table.

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ORGANIC COMPOUNDS (Continued)

No.	Crystalline form, color and index of refraction	Density g/ml	Melting point, °C	Boiling point, °C	Solubility in grams per 100 ml of		
					Water	Alcohol	Ether, etc.
2160	col. liq., 1.4398	1.299 ²	-112.4	101.6	i.	∞	∞ eth.
2161	col. liq., 1.4344 ²⁵	1.2580 ²		91.3	i.		
2162	col. liq., 1.428	1.222 ²	-20	73.3	i.		

For explanations and abbreviations see beginning of table.

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rather than systematic names, can make finding an entry a bit more difficult. There's a miniature gloss at the bottom of each page to help you find related compounds.

Butyl carbinol(n), at the bottom of Fig. 14, has an index number of 404. If you're familiar with the carbinol naming scheme for alcohols, it isn't much to translate that to 1-pentanol. The entry still comes *before* the B's because Amyl alcohol(n) is another common name for 1-pentanol. On the page where 1-pentanol would show up, there's *only* a gloss entry: 1-

Section 7

Table 7-4 (Continued)
PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS

No.	Name	Synonym	Formula	Beil. Ref.	Formula Weight
711	Benzoic acid		$C_6H_5 \cdot CO_2H$	IX-92	122.12
712	Na salt	sodium benzoate	$C_6H_5 \cdot CO_2Na \cdot H_2O$	IX-107	162.12

Benznaphthalide 765

Benzoic acid sulfamide 5671-3

Section 7

Table 7-4 (Continued)
PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS

No.	Name	Synonym	Formula	Beil. Ref.	Formula Weight
1040	Butyl amine (sec)		$(C_2H_5)(CH_3) : CH \cdot NH_2$	IV-160	73.14
1041	amine (<i>iso</i>)		$(CH_3)_2CH \cdot CH_2 \cdot NH_2$	IV-163	73.14
1057	bromide (<i>n</i>)	1-bromo-butane	$C_2H_5 \cdot CH_2 \cdot CH_2Br$	I-119	137.03
1058	bromide (<i>sec</i>)	2-bromo-butane	$C_2H_5 \cdot CHBr \cdot CH_3$	I-119	137.03
1059	bromide (<i>iso</i>)	1-Br-2-Me-propane	$(CH_3)_2CH \cdot CH_2Br$	I-126	137.03
1060	bromide (<i>tert</i>)	2-Br-2-Me-propane	$(CH_3)_3CBr$	I-127	137.03

Butyl borate 6117

Butyl carbinol (*iso*) 406Butyl carbinol (*tert*) 410

Butyl carbamide 1138-9

Butyl carbinol (*sec*) 411

Butyl carbitol 2232

Butyl carbinol (*n*) 404

Fig. 14 Sample entries from *Lange's Handbook of Chemistry*, 11th ed., J. Dean, copyright by McGraw-Hill, Inc., 1221 Avenue of the Americas, NY. Reprinted with permission.

Pentanol, 404. This brings you right back to *Amyl alcohol*(n). Since most textbooks and lab books are making it a *very big deal* these days to list none but the purest of pristine systematic nomenclature, you'd likely never expect the compounds to be listed this way, and that is a bit annoying. Even though you are missing out on a bit of the history in the field.

ORGANIC CHEMISTRY

Table 7-4 (Continued)
PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS

No.	Crystalline Form and Color	Specific Gravity	Melting Point °C.	Boiling Point °C.	Solubility in 100 Parts		
					Water	Alcohol	Ether
711	mn. pr.	1.316 ₄ ^{25°}	122.4; subl. > 100	250.0	0.21 ^{17.5°} ; 2.2 ^{75°}	46.6 ^{15°} , abs. al.	66 ^{15°}
712	col. cr.		-H ₂ O, 120		61 ^{25°} ; 77 ^{100°}	2.3 ^{25°} ; 8.3 ^{75°}	

Benzophenone oxide 6451

ORGANIC CHEMISTRY

Table 7-4 (Continued)
PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS

No.	Crystalline Form and Color	Specific Gravity	Melting Point °C.	Boiling Point °C.	Solubility in 100 Parts		
					Water	Alcohol	Ether
1040	col. lq.	0.724 ₂₀ ^{20°}	-104	66 ^{772mm}	∞	∞	∞
1041	col. lq.	0.732 ₂₀ ^{20°}	-85	68-9	∞	∞	∞
1057	lq.	1.275 ₂₀ ^{20°}	-112.4	101.6	0.06 ^{18°}	∞	∞
1058	lq.	1.261 ₂₀ ^{20°}	-112.1	91.3	l.		
1059	lq.	1.264 ₂₀ ^{20°}	-117.4	91.4	0.06 ^{18°}	∞	∞
1060	lq.	1.220 ₂₀ ^{20°}	-16.2	73.3; d. 210	0.06 ^{18°}	∞	∞

Butyl carbonate 1892-4

Butyl chlorocarbonate 1077-8

Butyl citrate 6119

Butyl cyanide (n) 6405

Butyl cyanide (iso) 6413

Butyl cyanide (tert) 6246

MERCK INDEX

(The Merck Index, Merck & Co., Inc., Rahway, New Jersey.) This handbook is concerned mostly with drugs and their physiological effects. But useful information exists concerning many chemicals. Because of the

1522

n-Butylbenzene

1526. *n*-Butyl Bromide. 1-Bromobutane. C_4H_9Br ; mol wt 137.03. C 35.06%, H 6.62%, Br 58.32%. $CH_3(CH_2)_3Br$. Prepd from *n*-butyl alc and a hydrobromic-sulfuric acid mixture: Kamm, Marvel, *Org. Syn.* vol. 1, 5 (1921); Skau, McCullough, *J. Am. Chem. Soc.* 57, 2440 (1935).

Colorless liquid. d_4^{25} 1.2686. bp_{760} 101.3° (mp -112°). n_D^{20} 1.4398. Insol in water; sol in alcohol, ether.

Page 216 Consult the cross index before using this section.

1093. Benzoic Acid. Benzenecarboxylic acid; phenylformic acid; dracrylic acid. $C_7H_6O_2$; mol wt 122.12. C 68.84%, H 4.95%, O 26.20%. Occurs in nature in free and combined forms. Gum benzoin may contain as much as 20%. Most berries contain appreciable amounts (around 0.05%). Excreted mainly as hippuric acid by almost all vertebrates, except fowl. Mfg processes include the air oxidation of toluene, the hydrolysis of benzonitrile, and the decarboxylation of phthalic anhydride: Faith, Keyes & Clark's *Industrial Chemicals*, F. A. Lowenheim, M. K. Moran, Eds. (Wiley-Interscience, New York, 4th ed., 1975) pp 138-144. Lab prepn from benzyl chloride: A. I. Vogel, *Practical Organic Chemistry* (Longmans, London α, 3rd ed, 1959) p 755; from benzaldehyde: Gattermann-Wieland, *Praxis des organischen Chemikers* (de Gruyter, Berlin, 40th ed. 1961) p 193. Prepn of ultrapure benzoic acid for use as titrimetric and calorimetric standard: Schwab, Wicher, *J. Res. Nat. Bur. Standards* 25, 747 (1940). Review: A. E. Williams in Kirk-Othmer *Encyclopedia of Chemical Technology* vol. 3 (Wiley-Interscience, New York, 3rd ed., 1978) pp 778-792.



Monoclinic tablets, plates, leaflets. d 1.321 (also reported as 1.266). mp 122.4°. Begins to sublime at around 100°. bp_{760} 249.2°; bp_{400} 277°; bp_{300} 205.8°; bp_{100} 186.2°; bp_{60} 172.8°; bp_{40} 162.6°; bp_{20} 146.7°; bp_{10} 132.1°. Volatile with steam. Flash pt 121-131°. K at 25°: 6.40×10^{-3} ; pH of satd soln at 25°: 2.8. Soly in water (g/l) at 0° = 1.7; at 10° = 2.1;

Fig. 15 Sample entries from the *Merck Index*, 10th edition.

nature of the listings, I've had to treat the explanations a bit differently than those for the other handbooks.

Entry: 1-Bromobutane (Fig. 15)

- 1. Top of page. 1522 *n*-Butylbenzene.** Just like a dictionary, each page has headings directing you to the first entry on that page. So, 1522 is not the page number but the compound number for *n*-Butylbenzene,

at 20° = 2.9; at 25° = 3.4; at 30° = 4.2; at 40° = 6.0; at 50° = 9.5; at 60° = 12.0; at 70° = 17.7; at 80° = 27.5; at 90° = 45.5; at 95° = 68.0. Mixtures of excess benzoic acid and water form two liquid phases beginning at 89.7°. The two liquid phases unite at the critical soln temp of 117.2°. Composition of critical mixture: 32.34% benzoic acid, 67.66% water: *see* Ward, Cooper, *J. Phys. Chem.* 34, 1484 (1930). One gram dissolves in 2.3 ml cold alc, 1.5 ml boiling alc, 4.5 ml chloroform, 3 ml ether, 3 ml acetone, 30 ml carbon tetrachloride, 10 ml benzene, 30 ml carbon disulfide, 23 ml oil of turpentine; also sol in volatile and fixed oils, slightly in petr ether. The soly in water is increased by alkaline substances, such as borax or trisodium phosphate, *see also* Sodium Benzoate.

Barium salt dihydrate, $C_{14}H_{10}BaO_4 \cdot 2H_2O$, *barium benzoate*. Nacreous leaflets. *Poisonous!* Soluble in about 20 parts water; slightly sol in alc. very sol in boiling water.

Calcium salt trihydrate, $C_{14}H_{10}CaO_4 \cdot 3H_2O$, *calcium benzoate*. Orthorhombic crystals or powder. d 1.44. Soluble in 25 parts water;

Cerium salt trihydrate, $C_{21}H_{15}CeO_4 \cdot 3H_2O$, *cerous benzoate*. White to reddish-white powder. Sol in hot water or hot alc.

Copper salt dihydrate, $C_{14}H_{10}CuO_4 \cdot 2H_2O$, *cupric benzoate*. Light blue, cryst powder. Slightly soluble in cold water, more in hot water; sol in alc or in dil acids with separation of benzoic acid.

Lead salt dihydrate, $C_{14}H_{10}PbO_4 \cdot 2H_2O$, *lead benzoate*. Cryst powder. *Poisonous!* Slightly sol in water.

Manganese salt tetrahydrate, $C_{14}H_{10}MnO_4 \cdot 4H_2O$, *manganese benzoate*. Pale-red powder. Sol in water, alc. Also occurs with $3H_2O$.

Nickel salt trihydrate, $C_{14}H_{10}NiO_4 \cdot 3H_2O$, *nickel benzoate*. Light-green odorless powder. Slightly sol in water; sol in ammonia; dec by acids.

Potassium salt trihydrate, $C_7H_5KO_2 \cdot 3H_2O$, *potassium benzoate*. Cryst powder. Sol in water, alc.

Silver salt, $C_7H_5AgO_2$, *silver benzoate*. Light-sensitive powder. Sol in 385 parts cold water, more sol in hot water; very slightly sol in alc.

Uranium salt, $C_{14}H_{10}O_6U$, *uranium benzoate*, *uranyl benzoate*. Yellow powder. Slightly sol in water, alc.

Toxicity: Mild irritant to skin, eyes, mucous membranes.

USE: Preserving foods, fats, fruit juices, alkaloidal solns, etc: manuf benzoates and benzoyl compds, dyes; as a mordant in calico printing: for curing tobacco. As standard in volumetric and calorimetric analysis.

THERAP CAT: Pharmaceutic aid (antifungal agent).

THERAP CAT (VET): Has been used with salicylic acid as a topical antifungal.

the first entry on page 216. The actual page number is at the bottom left of the page.

2. ***n*-Butyl Bromide**. Listed as a substituted butane with the systematic name given as a synonym.
3. ***C 35.06%***, ... Elemental analysis data; the percent of each element in the compound.
4. ***Prepd from.*** ... A short note on how 1-bromobutane has been prepared, and references to the original literature (journals).

5. **1.2686.** The tiny 25 over 4 makes this a specific gravity. Note that the temperatures are given with the **d** and not with the numerical value as in *Lange's* and the *CRC*.

Entry: Benzoic Acid (Fig. 15)

1. **Line 2. dracylic acid.** What a synonym! Label your benzoic acid bottles this way and no one will ever "borrow" your benzoic acid again.
2. **Lines 3–7.** Natural sources of benzoic acid.
3. **Lines 7–9.** Industrial syntheses of benzoic acid. These are usually not appropriate for your lab bench preparations.
4. **Lines 9–20.** References to the preparation and characteristics of benzoic acid in the original literature (journals).
5. **Structure.** A structural formula of benzoic acid.
6. **Lines 21–40. Physical data.** The usual crystalline shape, density (note *two* values reported.), sublimation notation, boiling point data, and so on. *K* at 25° is the ionization constant of the acid; the pH of the saturated solution (2.8 at 25°C) is given. The solubility data (*Soly*) are very complete, including water solutions at various temperatures, a bit about the phase diagram of the compound, and solubility in other solvents. Note that numerical data are given where possible.
7. **Lines 41–67.** Properties of some salts of benzoic acid.
8. **Line 68.** Toxicity data for benzoic acid.
9. **Lines 69–72.** Some commercial uses of benzoic acid.
10. **Lines 73–75.** Therapeutic uses, both human and veterinary, for benzoic acid.

If all the chemical entries were as extensive as the one for benzoic acid, this would be the handbook of choice. Because benzoic acid has wide use in medicine and food production, and it is very important to know the physical properties of drugs and food additives, a lot of information on benzoic acid winds up in the *Index*. 1-Bromobutane has little such use, and the size of the entry reflects this. Unfortunately, many of the compounds you come in contact with in the organic laboratory are going to be listed with about the same amount of information you'd find for 1-bromobutane, and not with the large quantities of data you'd find with benzoic acid.

THE ALDRICH CATALOG

(The Aldrich Catalog, Aldrich Chemical Co., Inc., Milwaukee, Wisconsin.) Not your traditional hard-bound reference handbook, but a handy book nonetheless. The company makes many compounds, some not yet listed in the other handbooks, and often gives structures and physical constants for them. Because Aldrich is in the business of selling chemicals to industry, many industrial references are given.

3

Entry: 1-Bromobutane (Fig. 16)

1. **1-Bromobutane.** Here it is listed *strictly* alphabetically as it is—with all the bromo-compounds—not as a butane, 1-bromo-, and only a cross reference as a butyl bromide.
2. **[109-65-9].** This is the Chemical Abstracts Service (CAS) Registry number. *Chemical Abstracts*, published by the American Chemical Society, is a listing of the abstract or summary written for any paper in the chemical literature. Every compound made gets a number. This makes for easy searching by computer as well as by hand.
3. **bp 100–104°.** Without a tiny superscript this is the boiling point at 760 torr.
4. **n_D^{20} 1.4390.** Index of refraction. The temperature (20°) modifies the n , rather than the number as in the *CRC*.

	Benzoic acid, 99+ %, GOLD LABEL, A.C.S. reagent	500g	17.20
	[65-85-0]	3kg†	80.65
24,238-1	C ₆ H ₅ CO ₂ H FW 122.12 mp 122-123° bp 249°		
★	Fp 250°F(121°C) <i>Beil.</i> 9,92 <i>Fieser</i> 1,49 <i>Merck</i>		
	<i>Index</i> 10,1093 <i>FT-IR</i> 1(2),186A <i>MSD Book</i> 1,160A		
	<i>RTECS#</i> DG0875000 <i>Disp.</i> A <i>IRRITANT</i>		
10,947-9	Benzoic acid, 99%, [65-85-0]	500g†	7.00
★	C ₆ H ₅ CO ₂ H	3kg†	31.00
23,988-7	1-Bromobutane, 99+ %, GOLD LABEL [109-65-9]	50g	15.75
★	(<i>n</i> -butyl bromide)		
	CH ₃ (CH ₂) ₃ Br FW 137.05 mp -112° bp 100-104°		
	n_D^{20} 1.4390 d 1.276 Fp 75°F(23°C) <i>Beil.</i> 1,119 <i>Merck</i>		
	<i>Index</i> 10,1526 <i>MSD Book</i> 1,236B <i>RTECS#</i> EJ6225000		
	<i>Disp.</i> D <i>FLAMMABLE LIQUID IRRITANT</i>		
B5,949-7	1-Bromobutane, 99%, [109-65-9] (<i>n</i> -butyl bromide)	500g	17.40
★	CH ₃ (CH ₂) ₃ Br	1kg	23.10

Fig. 16 Sample entries from the *Aldrich Catalog*, 1986–87.

5. ***d* 1.276.** The density in g/cc.
6. ***Fp* 75°F(23°C) Flash Point.** Above 75°F, a mixture of 1-bromobutane and air and a spark will go up like gangbusters. Watch out!
7. ***Beil.* 1, 119.** The Beilstein reference; Volume 1, page 119.
8. ***Merck Index* 10, 1526.** The *Merck Index*, 10th ed. reference; compound #1526 (Fig. 15).
9. ***MAS Book* 1, 236B.** A reference to the page location of the entry in the *Sigma-Aldrich Library of Chemical Safety Data*, Edition 1.
10. ***RTECS#* EJ6225000.** The reference number in the *Registry of Toxic Effects of Chemical Substances (RTECS)*. 1-Bromobutane is on the inventory of the Environmental Protection Agency (EPA) according to the Toxic Substances Control Act, PL9469, October 11, 1976 (TSCA).
11. ***Disp D.*** There are methods of disposal given in the *Aldrich Catalog*. Go to method D and throw 1-bromobutane out according to the rules. Remember, the methods given are for the disposal of large amounts of a single substance, as might be found in an industrial application. The rules for the disposal of the waste generated in your undergraduate laboratory may differ considerably.
12. ***Flammable liquid irritant.*** Yep, it sure is.

Note the differences in prices for the 99+% GOLD LABEL and the merely 99% 1-bromobutane. Before you buy, check on the use of the chemical. Normally, you can buy the least expensive grade of the chemical, and distill or recrystallize it yourself before you use it, if necessary.

Entry: Benzoic Acid (Fig. 16)

1. ***Fieser* 1, 49.** A reference to Fieser & Fieser's *Reagents for Organic Synthesis*, Volume 1, page 49. This multivolume series gives the syntheses and reactions of many organic compounds, along with references to the original literature.
2. †. Benzoic acid cannot be shipped by parcel post.
3. ***Beil.* 9, 92.** A reference to Beilstein, Volume 9, page 92.
4. ***FT-IR* 1(2)186A.** The Fourier-Transform Infra-Red spectrum of benzoic acid is in Edition 1, Volume 2, page 186A of *The Aldrich Library of FT-IR Spectra*.

NOT CLEAR—CLEAR?

One antonym for **clear** is **cloudy**. Another antonym for **clear** is **colored**. When you say you “obtained a clear liquid,” do you mean that it is not cloudy or that it is colorless?

Cloudiness usually means you’ve gotten water in your organic liquid. Colorless should be self-explanatory. You should always pair the turbidity and color designations:

“a clear, colorless liquid”

“a clear, blue liquid”

“a cloudy, colorless liquid”

“a cloudy, blue liquid”

I use clear to mean not cloudy, and *water-white* to mean not colored. Water-white is a designation found in the older chemical literature; **colorless** is more modern.

Is that clear?